Quantum Monte Carlo Calculations of Pion Inelastic Scattering

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Abstract

We show that the neutron and proton transition densities predicted by recent quantum Monte Carlo calculations for light nuclei are consistent with pion inelastic scattering. This provides a microscopic understanding of the enhancement factors for quadrople excitations, which were needed to describe pion inelastic scattering within the nuclear shell model of Cohen and Kurath.

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Quantum Monte Carlo (QMC) methods have been successfully developed to predict the properties of low-lying states of light nuclei starting with realistic two- and three-nucleon potentials [1]. While the reproduction of the energy spectra is the essential first step in such an effort, the dynamical content of the resulting nuclear wave functions must be tested against various reactions. This has been achieved so far mainly by considering electroweak processes [2,3]. In this paper we report on an additional test by using pion inelastic scattering.

Let us first briefly review the status of our understanding of pion inelastic scattering at medium energies(120 MeV $< E_{lab} <$ 300 MeV). Because of the excitation of the Δ resonance, the pion-nucleus interactions in this energy region are dominanted by the strong absorption mechanism. Consequently, the pion-nucleus inelastic scattering leading to discrete final nuclear states can be described by the distorted wave impulse approximation (DWIA). This has been well established [4–13] in very extensive investigations of the data from meson factories. Following the momentum-space approach [7], the inelastic scattering amplitude can be written as

$$T_{fi}(\vec{k}_0', \vec{k}_0) = \int d\vec{k}' \int d\vec{k} \chi^{(-)*}_{\vec{k}_0,f}(\vec{k}') U_{fi}(\vec{k}', \vec{k}) \chi^{(+)}_{\vec{k}_0}(\vec{k}) \,, \tag{1}$$

where the $\vec{k}$'s are pion-nucleus relative momenta in the $\pi-$nucleus center of mass frame, and the distorted waves $\chi^{(\pm)}$ are generated from an optical potential which is adjusted to fit the pion-nucleus elastic scattring.

The nuclear excitations are contained in the transition potential U_{fi}. It can be calculated from the πN scattering t-matrix and nuclear transition form factors. The details were given in Ref. [7]. To simplify the presentation, the spin-isospin variables will be suppressed here. Then the transition potential can be written as

$$U_{fi}(\vec{k}', \vec{k}) = t_{\pi n}(\vec{k}', \vec{k}, \omega_0) f^{-1/2}_{fi}(\vec{q}) + t_{\pi p}(\vec{k}', \vec{k}, \omega_0) f^{1/2}_{fi}(\vec{q}) \,, \tag{2}$$

where $\vec{q} = \vec{k}' - \vec{k}$, $t_{\pi n}(t_{\pi p})$ is an appropriately parameterized $\pi-$neutron (π-proton) scattering amplitude, and ω_0 is the collision energy calculated from using the fixed-scatterer approximation. With $t_3 = -1/2, 1/2$ denoting neutron and proton respectively, the nuclear transition form factors are defined by

$$f^{t_3}_{fi}(\vec{q}) = \int d\vec{r} e^{-i\vec{r}\cdot\vec{q}} \rho^{t_3}_{fi}(\vec{r}) \,, \tag{3}$$

with the transition densities defined by

$$\rho^{t_3}_{fi}(\vec{r}) = < \Psi_f \mid \frac{1}{A} \sum_{i=1,A} \delta(\vec{r} - \vec{r}_i) \frac{1 + 2t_3\tau_z(i)}{2} \mid \Psi_i > \,, \tag{4}$$

where τ_z is the z-component of the nucleon isospin operator, Ψ_i and Ψ_f are the initial and final nuclear states respectively. The transition dynamics can be better understood from the multipole expansion of transition densities

$$\rho^{t_3}_{fi}(\vec{r}) = \sum_{KM} \frac{1}{r^2} Y_{KM}(\hat{r}) < J_f M_f \mid J_i K M_i M > F^{fiK}_{K0,t_3}(r) \,, \tag{5}$$

Here we recall the notation of Ref. [7] to include possble spin transitions $S = 0, 1$ in $F^{fiJ}_{KS,t_3}(r)$, where K denotes the orbital angular momentum transition and $\vec{J} = \vec{K}+\vec{S}$ is the total angular momentum transfer.

In the DWIA study [7] for 1p-shell nuclei, the transition densities were calculated from the shell model of Cohen and Kurath [14]

$$F^{fiJ}_{KS,t_3}(r) = \sum_{\alpha\beta} A_{J(KS)t_3}(\alpha,\beta;fi)(4\pi j_\alpha)^{1/2} < (l_\alpha 1/2)j_\alpha \mid\mid [Y_K(\hat{r}) \times \sigma_S]_J \mid\mid (l_\beta 1/2)j_\beta > \times R_{n_\alpha l_\alpha}(r) R_{n_\beta, l_\beta}(r) \tag{6}$$

with $\sigma_0 = 1$, $\sigma_1 = \vec{\sigma}$, and

$$A_{J(KS)t_3}(\alpha,\beta;fi) =< \Psi_f \mid\mid [b^\dagger_{\alpha t_3} \times h^\dagger_{\beta t_3}]_{J[KS]} \mid\mid \Psi_i > \tag{7}$$

where $\alpha(n_\alpha, l_\alpha, j_\alpha)$ denotes the single particle orbitals, $R_\alpha(r)$ is the radial wave function, and $b^\dagger_\alpha$ and $h^\dagger_\beta$ are the creation operators for the particle and hole states respectively.

It was found that the pion inelastic scattering from 1p-shell nuclei can be described by using the above shell-model input only when the quadrople excitation component $J(KS) = 2(20)$ is enhanced by a factor $E_N \sim 2$. In Ref. [7], these enhancement factors were estimated from a systematic analysis of $B(E2)$ transitions from 1p-shell nuclei. For proton excitation, this enhancement factor is consistent with what is needed for explaining $B(E2)$ values. For $Z = N$ nuclei, one can assume that the neutron excitation also has the same enhancement because of isospin invariance. However, for the $N \neq Z$ nuclei, such as ^{7}Li, the enhancement factors for neutron excitations can not be obtained without making some additional assumptions. The predicted pion inelastic cross sections thus are not well justified theoretically. Furthermore, it would be desirable if the calculations do not include any enhancement factors. This however is very difficult, if not impossible, in practice within the shell model since the collective quardrople excitations can only be described by a very large model space.

In this work, we calculate the transition densities for a given multipolarity by using wave functions from the recent QMC calculations for light nuclei. The input, Eq.(6), to the DWIA calculations for pion inelastic scattering is then defined by the following matrix element

$$F^{fiJ}_{KS,t_3}(r) = \frac{< \Psi_{J_f M_f} \mid \sum_{i=1,A} \delta(r - r_i) r_i^K [Y_K(\hat{r}_i) \times \sigma_S]_{JM} \frac{1+2t_3\tau(i)}{2} \mid \Psi_{J_i M_i} >}{< J_f M_f \mid J_i J M_i M >} \tag{8}$$

The QMC calculations use a realistic Hamiltonian containing the Argonne v_{18} two-nucleon [15] and Urbana IX [16] three-nucleon potentials, which we refer to as the AV18/UIX model. Both variational (VMC) and Green's function (GFMC) Monte Carlo calculations have been made for light nuclei [1]. The AV18/UIX model reproduces the experimental binding energies and charge radii of ^{3}H, ^{3}He, and ^{4}He, in the numerically exact GFMC calculations, but underbinds ^{6}Li and ^{7}Li by 2–5%. The best variational Monte Carlo (VMC) energies are an additional 10% above the GFMC results. However, the known excitation spectra are well reproduced by both the VMC and GFMC calculations, as are the charge radii. The VMC and GFMC calculations also produce very similar one-body densities, while two-nucleon density distributions differ by less than 10%.

The VMC wave functions have been used successfully to describe the elastic and transition electromagnetic form factors for ^{6}Li [2] without introducing effective charges. They have also given an excellent absolute prediction for the spectroscopic factors in $^7\mathrm{Li}(e,e'p)$ reaction [3]. Consequently we expect the VMC wave functions to give a good estimate for the transition densities required in inelastic pion scattering.

The variational wave function for A=7 nuclei used here is the trial wave function, Ψ_T, that serves as the starting point for the GFMC calculations. It has the general form

$$|\Psi_T\rangle = \left[1 + \sum_{i<j<k} \tilde{U}^{TNI}_{ijk}\right] \left[\mathcal{S}\prod_{i<j}(1+U_{ij})\right] |\Psi_J\rangle \ , \tag{9}$$

where U_{ij} and $\tilde{U}^{TNI}_{ijk}$ are two- and three-body correlation operators and the Jastrow wave function $|\Psi_J\rangle$ is given by

$$|\Psi_J\rangle = \mathcal{A}\left\{ \prod_{i<j<k\le 4} f^c_{ijk} \prod_{i<j\le 4} f_{ss}(r_{ij}) \prod_{k\le 4} f_{sp}(r_{k5}) f_{sp}(r_{k6}) f_{sp}(r_{k7}) \right.$$
$$\left. \sum_{LS} \left(\beta_{LS[n]} \prod_{5\le l<m} f^{LS[n]}_{pp}(r_{lm}) |\Phi_7(LS[n]JMTT_3)_{1234:567}\rangle \right) \right\} \ . \tag{10}$$

The $\mathcal{S}$ and $\mathcal{A}$ are symmetrization and antisymmetrization operators, respectively. The central pair and triplet correlations $f_{xy}(r_{ij})$ and f^c_{ijk} are functions of relative positions only; the subscripts xy denote whether the particles are in the s- or p-shell. The $|\Phi_7(LS[n]JMTT_3)\rangle$ is a single-particle wave function with orbital angular momentum L, spin S, and spatial symmetry $[n]$ coupled to total angular momentum J, projection M, isospin T, and charge state T_3:

$$|\Phi_7(LS[n]JMTT_3)_{1234:567}\rangle = |\Phi_\alpha(0000)_{1234}\phi^{LS}_p(R_{\alpha 5})\phi^{LS}_p(R_{\alpha 6})\phi^{LS}_p(R_{\alpha 7})$$
$$\left\{ [Y_{1m_l}(\Omega_{\alpha 5}) Y_{1m'_l}(\Omega_{\alpha 6}) Y_{1m''_l}(\Omega_{\alpha 7})]_{LM_{L[n]}} \times [\chi_5(\tfrac{1}{2}m_s)\chi_6(\tfrac{1}{2}m'_s)\chi_7(\tfrac{1}{2}m''_s)]_{SM_S} \right\}_{JM}$$
$$\times [\nu_5(\tfrac{1}{2}t_3)\nu_6(\tfrac{1}{2}t'_3)\nu_7(\tfrac{1}{2}t''_3)]_{TT_3}\rangle \ . \tag{11}$$

Particles 1–4 are placed in an α core with only spin-isospin degrees of freedom, denoted by $\Phi_\alpha(0000)$, while particles 5–7 are placed in p-wave orbitals $\phi^{LS}_p(R_{\alpha k})$ that are functions of the distance between the center of mass of the α core and particle k. Different amplitudes $\beta_{LS[n]}$ are mixed to obtain an optimal wave function by means of a small-basis diagonalization. For the $(J^\pi;T) = (\frac{3}{2}^-;\frac{1}{2})$ ground and $(\frac{1}{2}^-;\frac{1}{2})$ first excited states of ^{7}Li the dominant amplitude is ^{2}P[3], with small admixtures of ^{2,4}P[21], ^{2,4}D[21], and ^{2}S[111] components. The $(J^\pi;T) = (\frac{7}{2}^-;\frac{1}{2})$ and $(\frac{5}{2}^-;\frac{1}{2})$ excited states are predominantly ^{2}F[3], again with small admixtures of ^{2,4}P[21] and ^{2,4}D[21] amplitudes. Mixing parameter values are given in Ref. [1].

The two-body correlation operator U_{ij} is defined as:

$$U_{ij} = \sum_{p=2,6} \left[\prod_{k\neq i,j} f^p_{ijk}(\mathbf{r}_{ik}, \mathbf{r}_{jk}) \right] u_p(r_{ij}) O^p_{ij} \ , \tag{12}$$

where the $O^{p=2,6}_{ij} = \boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j$, $\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j$, $\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j$, S_{ij}, and $S_{ij}\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j$. The six radial functions $f_{ss}(r)$ and $u_{p=2,6}(r)$ are obtained from two-body Euler-Lagrange equations with variational

parameters [17]. The f_{sp} and $f_{pp}^{LS[n]}$ correlations are similar to f_{ss} for small separations, but include parametrized long-range tails. The parameters used in constructing these two-body correlations, as well as the description of the three-body correlation operator $\tilde{U}_{ijk}^{TNI}$ and the operator-independent three-body correlations f_{ijk}^{c} and f_{ijk}^{p} are given in Ref. [1].

The quadrupole transition density,

$$\rho_{E2}^{t_3}(r) = \frac{\sqrt{2J_f+1}\langle \Psi_{J_f M_f} \mid \sum_{i=1,A} \delta(r-r_i) r_i^2 Y_2^M(\hat{r}_i) \frac{1+2t_3\tau(i)}{2} \mid \Psi_{J_i M_i}\rangle}{\langle J_f M_f \mid J_i 2 M_i M\rangle} \ , \tag{13}$$

and the initial and final state wave function normalizations are evaluated using 40 000 Monte Carlo samples for transitions from the ground state to the lowest three excited states of ^{7}Li. The neutron and proton transition densities for all three transitions are shown in Fig. 1. The integrated $B(E2\uparrow, t_3)$ values,

$$B(E2\uparrow, t_3) = \frac{\mid \int \rho_{E2}^{t_3}(r) d^3r \mid^2}{2J_i+1} \ , \tag{14}$$

are shown in Table I, where they are compared to the experimental proton values obtained from (e,e') scattering and Coulomb excitation [18].

We see from Fig.1 and Table 1 that the predicted differences between the neutron and proton excitations are very significant. Such differences can be most effectively verified by using an important characteristic of pion scattering at energies near the Δ excitation. At a typical energy $E_\pi = 164$ MeV, one finds that the πN amplitude in Eq.(2) has an interesting ratio $\mid t_{\pi^+p}/t_{\pi^+n} \mid = \mid t_{\pi^-n}/t_{\pi^-p} \mid \sim 3$. Consequently, the π^+ scattering is dominanted by the proton excitations while π^- scattering is dominanted by neutron excitations. The agreement with both the π^+ and π^- data will be a nontrivial test of the predicted wave functions. Thus the present study is complementary to that of Ref. [2] using electron scattering which mainly probes the proton excitations.

We have performed DWIA calculations for π^+ and π^- inelastic scattering from ^{7}Li. The pion optical potential and the πN t-matrix were taken from Ref. [7]. The considered final states are $(J^\pi;T) = (\frac{1}{2}^-;\frac{1}{2})$ at 0.478 MeV, $(\frac{7}{2}^-;\frac{1}{2})$ at 4.63 MeV, and $(\frac{5}{2}^-;\frac{1}{2})$ at 6.68 MeV. As found in Ref. [7], these states are excited predominantly by the quadrapole transition $J(KS) = 2(20)$. From Eqs.(8) and (13), the transition densities needed for our DWIA calculations can be obtained from $F_{20,t_3}^{fi,2}(r) = \rho_{E2}^{t_3}(r)/\sqrt{2J_f+1}$. With the transition densities calculated from QMC, there are no adjustable parameters in our calculations. The results are shown in Fig. 2. We see that the predicted cross sections (solid curves) are in excellent agreement with the data. In the same figure, we also show the contributions from proton excitations. The agreement with both the π^+ and π^- data is evidently due to the delicate interplay between the neutron and proton excitations. If the shell model input given in Ref. [7] is used without the enhancement factors $E_n = 1.75$ and $E_p = 2.5$ for the quadrapole transition ($J(KS) = 2(20)$), the predicted cross sections will be a factor of about 5 lower than the data for all of the cases considered here.

In conclusion, we have performed a DWIA calculation of pion inelastic scattering from ^{7}Li using the nuclear transition densitions predicted by the recent QMC calculations for light nuclei starting with realistic two-nucleon and three-nucleon potentials. The predicted cross sections are in excellent agreement with the data at 164 MeV. In contrast with the previous

calculations using nuclear shell model, the calculation does not include any enhancement factors. Because of the strong isospin dependence of the πN scattering t-matrix, the present investigation has probed critically the predicted neutron transition densities which were not well tested in the study using electron scattering. Our results suggest that the wave functions predicted by the QMC calculations are accurate for investigating various nuclear reactions. It is highly desirable to extend the present work to re-investigate the very extensive data of pion-nucleus scattering on 1p-shell targets and other more complex processes such as pion absorption and double-charge-exchange reactions. With the nuclear correlations correctly accounted for by using the wave functions predicted by QMC calculations, one now can hope to resolve many long-standing problems in intermediate-energy pion-nucleus reactions.

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TABLES

TABLE I. $B(E2\uparrow, t_3)$ values in fm^4 for different transitions from the $\frac{3}{2}^-$ ground state of ^{7}Li. Experimental values are from Ref. [18]. Experimental uncertainties and Monte Carlo sampling errors are given in parentheses.

	Experiment	QMC	
J_f	p	p	n
$\frac{1}{2}^-$	7.2(7)	5.9(2)	17.0(6)
$\frac{7}{2}^-$	15.5(8)	12.6(3)	33.0(8)
$\frac{5}{2}^-$	4.1(2.0)	2.2(1)	4.9(2)

FIGURES

FIG. 1. The transition densities, $\rho_{E2}^{n,p}$, for ^{7}Li.

FIG. 2. Differential cross sections for $^7\mathrm{Li}(\pi,\pi')$ scattering. The data are taken from Ref.[19].

Fig. 1 Lee & Wiringa

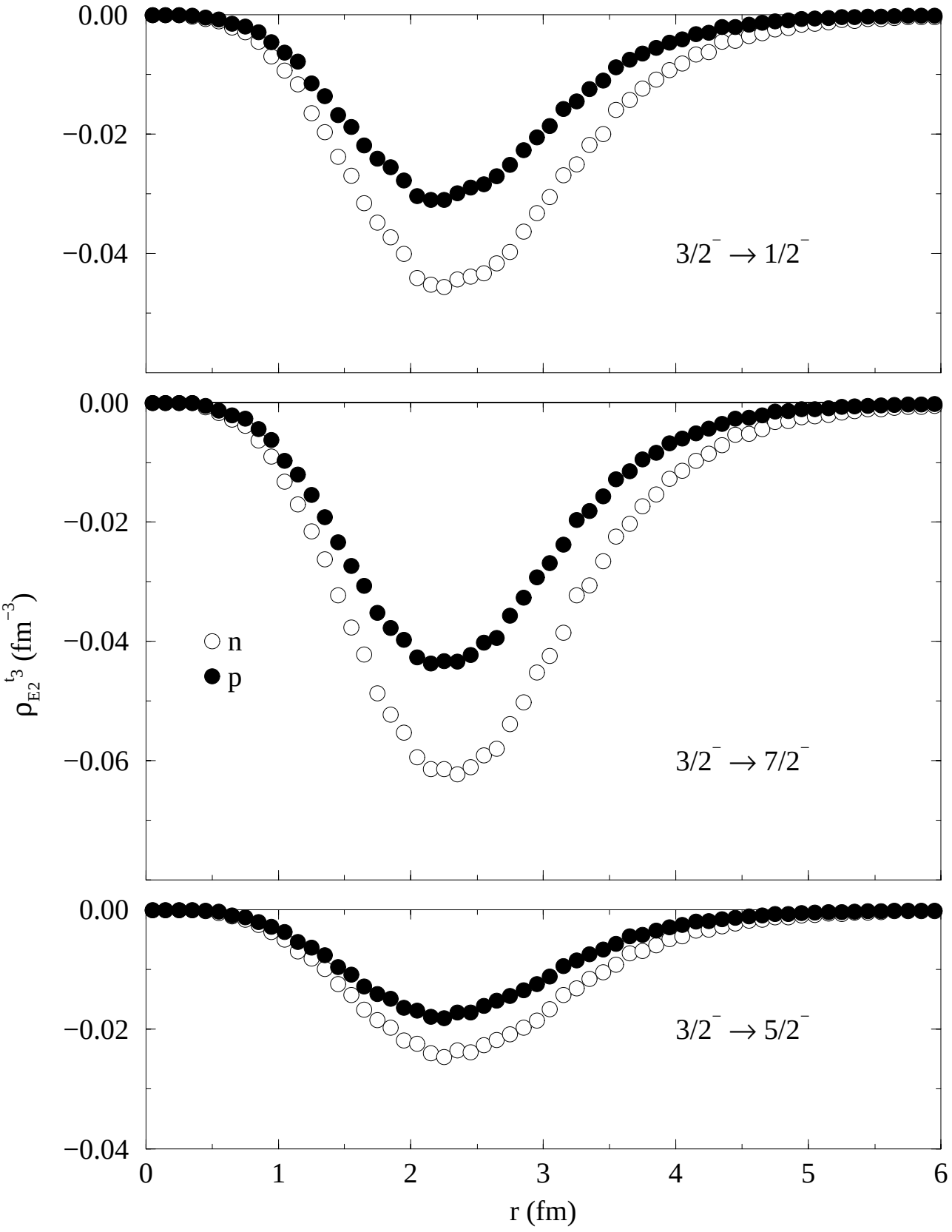

Fig. 2 Lee & Wiringa